STAT 401 Chapter 10.2–10.4

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1 Identifying outlying X observations: leverage h_{ii}

1.1 What can go wrong?

With a one-predictor model, we can demonstrate three noteworthy problems of a certain data point (x_i, y_i) :

- 1. Outlying in terms of X
 - (a) y_i is away from the "expected" Y at this x_i as is indicated by the trend suggested by the other data points.
 - (b) (x_i, y_i) is "in the trend" but is far from other data points.
- 2. Within range in terms of X
 - but Y is "out of trend"

If there are two predictors, on a X_1 - X_2 scatter plot it is easy to see whether a data point is outlying in terms of X, but it is harder to check Y (a 3-D plot would be needed).

With three or more predictors, the above are still the problems to check for, but it is not easy to do by graphics. Effective, easy-to-interpret numerical measures are needed. The secret is in the "hat" matrix.

1.2 "Leverage" value in terms of X

The outlying-ness of X of the ith observation is indicated by the ith diagonal element of \boldsymbol{H} , h_{ii} , called <u>leverage</u>. Recall $\boldsymbol{H} = \boldsymbol{X} (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T$. Its ith diagonal element is

$$h_{ii} = \mathbf{x}_i'(\boldsymbol{X}'\boldsymbol{X})^{-1}\mathbf{x}_i$$

where \mathbf{x}_i (a column vector) is the transpose of the *i*th row of \mathbf{X} . Note: \mathbf{x}_i has a leading 1 if the model contains intercept.

Note: h_{ii} indicates the "outlying-ness" in terms of X. It is natural that this measure does not involve Y. This indicator can be examined even before Y is available.

Properties of h_{ii} :

$$0 \le h_{ii} \le 1, \quad \sum_{i=1}^{n} h_{ii} = p$$

where n is sample size and p is df of the model, i.e. number of β 's and number of rows (or columns) in the design matrix X and the hat matrix H.

Example Figure 10.6, page 398.

Example Figure 10.7, page 399.

1.3 Interpretation

- 1. h_{ii} somehow measures the distance of \mathbf{x}_i from the center of all the X vectors (one vector for each case, or "observation", or "data point").
- 2. A large h_{ii} implies large leverage on model estimation. We don't want any observation to have much larger leverage than others. Indeed, in experimental studies, one strives to lay out X (before proceed to spend money and time measuring Y) such that no case has exceptionally large leverage on the model estimation.
- 3. How large is too large? The average leverage is

$$\overline{h} = \frac{\sum h_{ii}}{n} = \frac{p}{n}$$

Rule of thumb: when $n \gg p$, a h_{ii} that is $> 2\overline{h}$ or > 0.5 is suspicious.

4. Although a high-leverage point is influential on the model estimation, its Y is not necessarily "out of trend" in a particular dataset. However, imagine its Y observation is indeed in disagreement with the trend suggested by the other cases. Then the strong influence on the model estimation exerted by this data point will show: it will "pull" the regression line towards itself.

Also see comment 1 on the top of page 399. (The comment is not totally accurate. Take it informally.)

5. Although it's convenient to remember h_{ii} with reference to the hat matrix \mathbf{H} , this measure really revolves

around $(\mathbf{X}^T \mathbf{X})^{-1}$, not \mathbf{H} . Here's how we can apply the idea to a \mathbf{x} that is not in the set of model-building points.

Suppose we apply the fitted model to a new predictor vector \mathbf{x}_* . Is the model applicable at this \mathbf{x}_* ? Check whether

$$h_* = \mathbf{x}'_* (\mathbf{X}' \mathbf{X})^{-1} \mathbf{x}_*$$

is notably larger than the leverages of the available data points. The above empirical rules may be used. If h_* is too big, it suggests we are <u>extrapolating</u> the model too much.

2 Identifying outlying Y observations: residuals

Using h_{ii} we can basically identify the data points that are outlying in terms of X. Remaining data points that are problematic are those whose X is within the range of the other X's but whose Y is "out of trend".

We identify problematic Y through residuals. Obviously, a large residual is bad. However, the "raw residuals" have limitations. Consider data points close to the "center" of the "data cloud" and those on the outskirts. A fitted model fits the central part best, meaning $E(\hat{Y})$ in the central part has small variance than on the outskirts. In other words, the residuals in the central part have small variance than on the outskirts. Whether a residual is "large" should be measured with its expected variation in mind, that is, using its standard deviation as the unit of distance (from its expected value, 0).

The residual vector is

$$e = Y - \hat{Y} = (I - H)Y$$

Recall

$$E(\mathbf{e}) = \mathbf{0}, \quad \text{var}(\mathbf{e}) = \sigma^2(\mathbf{I} - \mathbf{H}), \quad s^2(\mathbf{e}) = s^2(\mathbf{I} - \mathbf{H})$$

where s^2 is the MSE. For an individual residual,

$$e_i = y_i - \hat{y}_i$$

we have

$$E(e_i) = 0$$
, $var(e_i) = \sigma^2(1 - h_{ii})$, $s^2(e_i) = s^2(1 - h_{ii})$

Note that a larger h_{ii} results in smaller residual variance.

Studentized residuals

Standardize the residual:

$$\frac{e_i - E(e_i)}{\operatorname{var}(e_i)} = \frac{e_i}{\sigma(e_i)} = \frac{e_i}{\sigma\sqrt{1 - h_{ii}}} \sim N(0, 1)$$

However, we don't know σ^2 ! Easy. Plug in the estimate:

$$e'_{i} = \frac{e_{i}}{s\sqrt{1 - h_{ii}}} = \frac{y_{i} - \hat{y}_{i}}{s\sqrt{1 - h_{ii}}}$$

If the model is "right", then e_i' has a t distribution with n-p df.

If the *i*th observation is really bad (e.g. having a large h_{ii}), it will make the model fitting bad and the estimate of s^2 not quite right. We remove this data point and re-fit the model with the remaining n-1 observations. Let the new fitted value be $\hat{y}_{(i)}$. Then define

$$e_i^* = \frac{y_i - \hat{y}_{(i)}}{\sqrt{\text{var}(y_i - \hat{y}_{(i)})}}$$

This is called a "studentized" residual. (The terminology is not universally adopted. Some call this a "jackknifed" residual. KNNL calls it "studentized deleted" residual.))

Fortunately, we do not need to actually remove the ith observation and refit a model. We have the following relation:

$$e_i^* = e_i \left(\frac{n-p-1}{(1-h_{ii})(n-p)s^2 - e_i^2} \right)^{1/2}$$

Of course, $(n-p)s^2$ is equal to SSE of the model fitted using all the observations.

It is usually better to compare studentized residuals rather than residuals. In particular, we recommend making normal probability plots using these residuals instead of the "raw" residuals.

 t_i^* follows a t distribution with n-p-1 df. This fact can be use to formally test whether a particular t_i^* is "large", i.e. significantly nonzero.

3 Identifying influential cases: Cook's distance

This time we identify influential cases, considering both X and Y. The "influence" is on the fitted model and fitted

values for all the observations. There are various measures. We'll take Cook's distance as an example.

Influence of the ith case on all n fitted values can be measured by

 $D_i = \frac{\sum_{j=1}^{n} (\hat{y}_j - \hat{y}_{j(i)})^2}{p \, s^2}$

where \hat{y}_j is the fitted value for the jth case in the model that is fitted using all n observations, $\hat{y}_{j(i)}$ is the fitted value for the jth case in the model that is fitted using all but the ith observation, and s^2 is the estimate of σ^2 in the model fitted using all observations.

Again, we don't need to do delete-one-and-refit, because

$$D_i = \frac{e_i^2}{p \, s^2} \frac{h_{ii}}{(1 - h_{ii})^2}$$

Therefore D_i increases as e_i and h_{ii} increases.

How do we judge the magnitude of D_i ? Use a F(p, n - p) distribution. Rule of thumb: if

$$D_i > F(0.5; p, n - p)$$

then the models fitted with and without the *i*th case are quite different. Recall F(0.5; p, n - p) is the median (50th percentile) of the F(p, n - p) distribution.

4 Computation

R has a number of functions for linear model diagnostics. These functions are grouped into a couple of help pages. If you type

> ?influence

you'll see help on several. If you type

> ?influence.measures

you'll see several others.

In the help page of a R function, the Value section tells you what the returned values are. Usually the returned object is a list with multiple components, and the Value section explains the meaning of each component. Another very useful section is See als, which points you to related functions.

```
> data <- read.table('USCrime.txt', header = TRUE)</pre>
> # 'R' is the reponse (crime rate).
> # We'll focus on the following predictors:
> # Age: number of male aged 14--24 per 1000 population
> # Ed: mean # of years of schooling
> # Ex0: per capita expenditure on police by government
          state population
> # U1: unemployment rate of urban males
          median family goods
> data <- data[, c('R', 'Age', 'Ed', 'Ex0', 'N', 'U1', 'W')]</pre>
> n <- nrow(data)</pre>
> print(n)
[1] 47
> myfit <- lm(R ~ ., data)</pre>
influence(myfit) and influence.measures(myfit) are com-
prehensive diagnostics; each returns a bunch of things. For
now, the specialized functions hatvalues, rstudent, and
cooks.distance suffice.
> # 'h_ii', or 'leverage' for each observation:
> print(hatvalues(myfit))
                     2
                                                       5
0.08218113 0.07512489 0.18944838 0.37821056 0.11393729 0.19959197 0.12093818
                     9
                               10
                                           11
                                                      12
                                                                  13
0.26461410 0.09019724 0.08643382 0.17215992 0.09924435 0.13531582 0.13013059
                    16
                               17
                                           18
                                                      19
                                                                  20
0.08434201 0.14161961 0.07745114 0.14170822 0.09335966 0.14374565 0.07114259
                                           25
                               24
                                                      26
0.19336522 0.09386727 0.20301930 0.19475315 0.35104388 0.10204543 0.10655219
                    30
                               31
                                           32
                                                      33
0.35202557 0.16063684 0.17313680 0.15748635 0.06375603 0.06759911 0.19430798
                                           39
                                                      40
0.16404292 0.24882370 0.11411457 0.08476158 0.12944923 0.18458990 0.06630050
                               45
        43
                    44
                                           46
0.15498044 0.10225807 0.23019163 0.11767407 0.09832115
> # Studentized residuals:
> rst <- rstudent(myfit)</pre>
> print(rst)
 0.18750262 1.74116483 0.32919051 1.30560757 -0.22604851 -1.17554343
```

```
10
                                                            11
                                                                         12
 1.12748034
             1.46385169
                          0.14042536 -0.58454298 2.89075383
                                                                0.65511836
         13
                      14
                                                            17
                                                                         18
                                   15
                                               16
-0.37151527
             0.09887924
                          0.50136337
                                       0.29648074 -1.12000785 -1.10227367
                                   21
                                                            23
         19
                      20
                                               22
-2.24807155
             0.55363681
                          0.45256806 -1.25074265
                                                   1.85759020
                                                                0.37676139
         25
                      26
                                   27
                                               28
                                                            29
                                                                         30
-0.34318578
             1.30841708 -1.12936378
                                       0.54994941 -2.82298138 -0.60037956
         31
                      32
                                   33
                                               34
                                                            35
                                                                         36
                          1.29075802 -0.11255729 -0.90872368
-0.84993786 -0.14109491
                                                                0.17639655
         37
                      38
                                   39
                                               40
                                                            41
             0.26195305
                          0.52944112
-0.59788329
                                       0.71627309 -0.12843619 -0.43381109
         43
                                   45
                                                            47
                                               46
-0.70249794 -0.13261485
                         0.15882463 -1.61990420 -0.42133318
> # Make a normal probability plot.
> pdf(file = 'part13-rstud-qq.pdf', width = 5, height = 5)
> qqnorm(rst, main = 'Norm QQ plot of studentized residuals')
> qqline(rst)
> dev.off()
X11
  2
> # Cook's distance of each case:
> print(cooks.distance(myfit))
                         2
                                       3
0.0004608248 \ 0.0334784992 \ 0.0037008128 \ 0.1455572954 \ 0.0009614649 \ 0.0487622972
           7
                         8
                                       9
                                                    10
                                                                 11
                                                                               12
0.0248158527 0.1070925580 0.0002862958 0.0046955401 0.2096962052 0.0068530286
                        14
                                      15
                                                    16
0.0031536062 0.0002142516 0.0033707228 0.0021200992 0.0149495799 0.0285044559
                                                    22
                                                                 23
                                                                               24
                        20
                                      21
0.0675029581 \ 0.0074806489 \ 0.0022864985 \ 0.0528268457 \ 0.0481171487 \ 0.0052788802
                                                    28
                                      27
0.0041610393\ 0.1299805808\ 0.0205649809\ 0.0052442218\ 0.5267213560\ 0.0100149525
                        32
                                      33
                                                    34
0.0217598849 \ 0.0005449597 \ 0.0159423310 \ 0.0001345370 \ 0.0285747833 \ 0.0008939324
          37
                        38
                                      39
                                                    40
                                                                               42
0.0171916490 0.0012928387 0.0037764803 0.0110327573 0.0005469157 0.0019485777
                                      45
                                                    46
0.0130959356 0.0002933810 0.0011044833 0.0480449352 0.0028233932
```

Norm QQ plot of studentized residuals

